Glycine ethyl ester

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459-7	'3-4	DTXSID901	9	664

Model Performance

_			
N	Model	Data	

Weighted KNN model

5-fold CV (75	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: -1.38

Global applicability domain: Inside

Local applicability domain index: 5.51e-01

Confidence level: 5.03e-01

Nearest Neighbors from the Training Set

Image not found

N-Methylglycine Measured: -2.78 Predicted: -2.19 Image not found

Diethanolamine Measured: -1.43 Predicted: -1.46 Image not found

Glycidol

Measured: -0.950 **Predicted:** -0.792

Image not found

N-Methylethanolamine Measured: -0.940 Predicted: -1.27 Image not found

2-Hydroxyethyl acrylate Measured: -0.210 Predicted: -0.0439